Optical constants (n, k) extraction from R, T measurements in organic thin film

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The characterization and modeling of Organic PhotoVoltaic (OPV) devices, generally composed of several layers of organic materials, typically requires an accurate determination of optical constants (n,k) [1]. Several approaches have been proposed to this aim, mostly using spectrophotometric measurements, such as ellipsometry [2] and reflectance and transmittance [3]. The real challenge for both techniques is the n and k extraction from measurements, especially when n and k are potentially of the same order of magnitude, and/or strongly varying with the wavelength, as in most organic materials used in OPV [4]. Indeed, for these materials, the simplest extraction techniques cannot be used. The “envelope” method [5] for example is limited to low absorbing materials. Moreover, multi-wavelength approaches usually require to know a-priori an equation for the dispersion model ([6]) (Cauchy equations, Sellmeier relations or a limited number of Lorentz oscillators). In consequence, a brute-force numerical inversion method has to be use to deduce (n,k) from measurements, which is known to lead to multiple solutions [7], requiring additional information to select the true (n,k) value from all multiple solutions.
The aim of this paper is to propose an original and complete methodology to extract n and k from R, T measurements without making any a-priori assumption. The proposed methodology is summarized in the following. 1/ R, T measurements are first performed on the substrate (typically an optical glass) 2/ As in [5], two samples are processed, featuring the same material, but two different thicknesses, accurately measured. 3/ Transmittance and reflectance measurements are performed thanks to a Perkin Elmer lambda 900 spectro-photometer. 4/ several techniques are performed to deduce (n,k) from measurements. First of all, approximated (n,k) values are extracted from “incoherent” formulas (ray optics). Even if this approach is in principle inaccurate in thin layers featuring strong interference effects, it does not suffer from multiple solutions, and usually gives good guess values for more rigorous approaches, especially for thick or strongly absorbing layers. Then, for ultra-thin layers (ne << λ), we use the brute-force numerical inversion method on each sample, as in this case, the number of multiple solutions is limited. The true (n,k) is deduced by confronting multiple solutions obtained on both samples. For thicker layers, we have developed a new inversion scheme that uses simultaneously the measurements performed at different thicknesses. This approach makes easier the determination of true (n,k) value from multiple solutions than the previous one. Figure 1 shows an example of extracted (n,k) obtained on P3HT deposited by spin coating on a glass substrate, compared to data found in the literature for similar material.

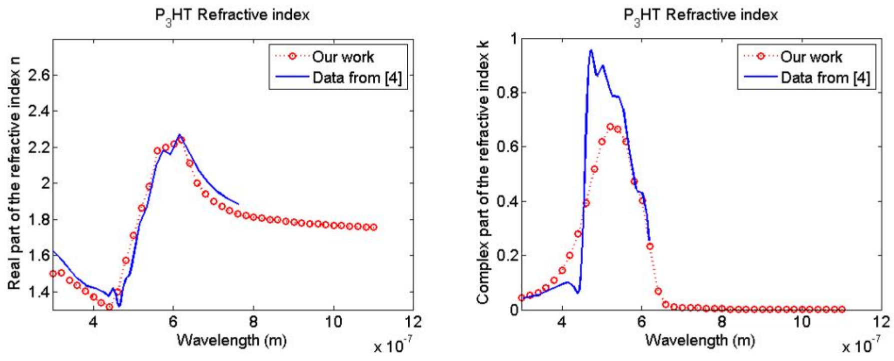

Figure 1 Real refractive index n (left image) and complex refractive index k (right) of P3HT samples

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